

# Quantum Numbers and Electronic Configuration

The purpose of quantum numbers and electronic configuration is to determine the ground state organization of electrons for any element. It can also be used to determine the arrangement of electrons in ions and excited state atoms. The ground state is the most stable, i.e. lowest energy, arrangement of electrons around a nucleus. Excited states are less stable, higher energy, alternative organizational states. All elements always adopt their ground configuration unless they undergo physical interaction with light or chemical reaction with another element. Quantum numbers explain the procedure by which the electronic configuration is determined. Quantum numbers can be compared to a zip code used by the Postal Service to determine the location a letter is to be sent; in the atomic case, quantum numbers determine the location an electron is to be sent.

## Quantum Numbers

There are four quantum numbers, each with a distinct role in determining electron configuration.

First Quantum Number--> also called Principal Quantum Number --> symbolized by 'n'  
allowed values for n = all integer values between 1 and 7 (i.e. 1, 2, 3, 4, 5, 6, 7)  
n corresponds to the Period Number in the Periodic Table of Elements  
n defines orbitals; lower value for n means electrons circulate closer to nucleus

Second Quantum Number--> also called Angular Quantum Number --> symbolized by 'l'  
allowed values for l = all integer values between 0 and n-1 (i.e. 0, 1, 2, 3, 4, 5, 6)  
in actual practice, only l = 0, 1, 2, 3 are used (on theoretical grounds, l = 4, 5, 6 will never be occupied because resulting atom will necessarily be unstable)  
l defines suborbitals; each suborbital has a characteristic shape indicating the manner in which an electron can move around a nucleus.

l = 0 --> called s suborbital, where s stands for spherical --> an electron in an s suborbital will travel a spherical 3D path around a nucleus

l = 1 --> called p suborbital, where p stands for perpendicular --> an electron in a p suborbital will move along a 3D coordinate axis around a nucleus; the path will look like a figure eight (8)

l = 2 --> called d suborbital, where d stands for diagonal --> an electron in a d suborbital will move between two of the 3D coordinate axes around a nucleus; for most d suborbitals, the path will look like a four leaf clover or two eights connected in the middle

l = 3 --> called f suborbital, where f stands for functional --> an electron in an f suborbital will move in a path in 3D space defined by a complex mathematical function

Third Quantum Number--> also called Magnetic Quantum Number --> symbolized by 'm'  
allowed values for m = all integer values between 0 and  $\pm l$  (i.e. 0,  $\pm 1$ ,  $\pm 2$ ,  $\pm 3$ )  
m defines the number of suborbitals of each type exist in atom; the value of m is unimportant; rather, it is the number of m values that determines the suborbital number

if l = 0, m = 0 only --> since there is only one m value, there is only one l = 0, or s, suborbital

if l = 1, m = 0,  $\pm 1$  only --> since there are three possible m values (0, +1, -1), there are three possible l=1, or p, suborbitals

if  $l = 2$ ,  $m = 0, \pm 1, \pm 2$  only --> since there are five possible  $m$  values (0, +1, -1, +2, -2), there are five possible  $l = 2$ , or d, suborbitals

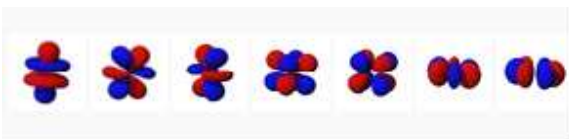
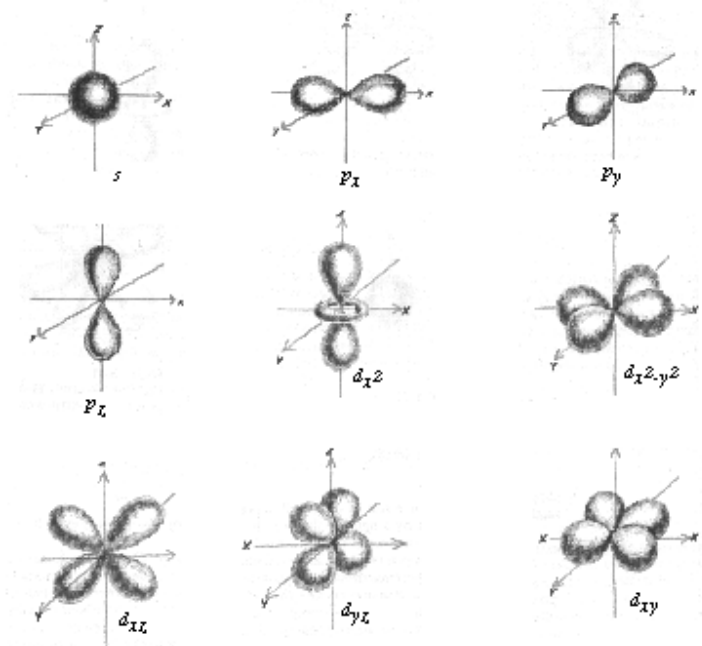
if  $l = 3$ ,  $m = 0, \pm 1, \pm 2, \pm 3$  only --> since there are seven possible  $m$  values (0, +1, -1, +2, -2, +3, -3), there are seven possible  $l = 3$ , or f, suborbitals

Fourth Quantum Number --> also called Spin Quantum Number --> symbolized by 's' (unfortunate symbolism; do NOT confuse with s suborbital)

allowed values for  $s = \pm 1/2$  only; values for  $n, l$ , and  $m$  do not affect values for  $s$

**students are not asked to draw or name specific suborbitals on AP exams**

Directional characteristics of s, p and d orbitals



$$f_z^3 \quad f_{xz}^2 \quad f_{yz}^2 \quad f_{xyz} \quad f_{z(x^2-y^2)} \quad f_{x(x^2-3y^2)} \quad f_{y(3x^2-y^2)}$$

Pauli Exclusion Principle --> no two electrons in the same atom can possess the same four quantum numbers ( $n, l, m, s$ )

## Electron Configurations

With quantum numbers in hand, the electron configuration of any element depends on the total number of electrons present, which can be determined from the atomic number. Electron placement is determined by application of the quantum numbers to the Pauli Exclusion Principle starting with the lowest energy orbital. The lowest energy orbital is closest to the nucleus in order to maximize proton-electron attractive force.

(a) First Cases:  $n = 1$  means  $l = 0$  means  $m = 0$  and  $s = \pm 1/2$

only possible sets of quantum numbers are  $(1, 0, 0, +1/2)$  and  $(1, 0, 0, -1/2)$

only at most two electrons can fit in the single s suborbital within the first orbital

${}^1_1\text{H} = 1s^1$  where 1 stands for orbital n, s stands for suborbital s, <sup>1</sup> stands for 1 electron

${}^2_2\text{He} = 1s^2$  where 1 stands for orbital n, s stands for suborbital s, <sup>2</sup> stands for 2 electrons

With 2 electrons assigned, no more electrons can fill s suborbital; 1p suborbitals cannot exist because a p suborbital means  $l=1$ , and this is impossible if  $n = 1$  and  $l$  can have a maximum value of  $n-1$  per quantum number rules for assignment of allowed values

(b) Second Cases:  $n = 2$  means  $l = 0, 1$  means  $m = 0, \pm 1$  and  $s = \pm 1/2$

possible quantum numbers sets are  $(2, 0, 0, +1/2)$  and  $(2, 0, 0, -1/2)$ , or 2s suborbitals

$(2, 1, 0, +1/2)$  and  $(2, 1, 0, -1/2)$  ----\

$(2, 1, +1, +1/2)$  and  $(2, 1, +1, -1/2)$  ----|--> or 2p suborbitals

$(2, 1, -1, +1/2)$  and  $(2, 1, -1, -1/2)$  ----/

Just as a single s suborbital can hold 2 electrons maximum, three p suborbitals can hold 6 electrons maximum. In general, *the maximum number of electrons is twice the number of suborbitals because quantum number s can have two values*. Therefore, the five d suborbitals can hold ten electrons maximum and the seven f suborbitals can hold fourteen electrons maximum, as shown below.

${}^3_3\text{Li} = 1s^2 2s^1$  Lithium starts with same configuration as previous element (He) and adds one electron. The 2s suborbital is filled before the 2p suborbital because  $l=0$  is smaller than  $l=1$ , which means a lower energy state

${}^4_4\text{Be} = 1s^2 2s^2$

${}^5_5\text{B} = 1s^2 2s^2 2p^1$  since all 2 p orbitals are equivalent, it doesn't matter whether this partially occupied suborbital is  $p_x$ ,  $p_y$ , or  $p_z$

${}^6_6\text{C} = 1s^2 2s^2 2p^2$  once a single electron is put in a 2p suborbital, the second electron will enter a different 2p suborbital in order to minimize electron-electron repulsive force

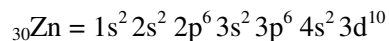
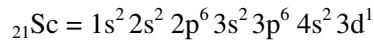
${}^{10}_{10}\text{Ne} = 1s^2 2s^2 2p^6$  with this configuration, the  $n = 2$  orbital (the 2nd period) is complete

(c) Third Cases:  $n = 3$  means  $l = 0, 1, 2$  means  $m = 0, \pm 1, \pm 2$  and  $s = \pm 1/2$

Without going through all the possibilities, the 3s and 3p suborbitals have quantum number sets identical to those listed in (b) with the only change being  $n = 3$  instead of  $n = 2$ . The possible 3d suborbital quantum number sets are:

(3, 2, 0, + 1/2) and (3, 2, 0, -1/2)  
 (3, 2, +1, + 1/2) and (3, 2, +1, -1/2)  
 (3, 2, -1, + 1/2) and (3, 2, -1, -1/2)  
 (3, 2, +2, + 1/2) and (3, 2, +2, -1/2)  
 (3, 2, -2, + 1/2) and (3, 2, -2, -1/2)

By looking at the Periodic Table, period 1 (n = 1) has only 2 elements; periods 2 and 3 (n = 2, 3) have 8 elements each. Period 4 (n = 4) begins with  $_{19}\text{K}$  and  $_{20}\text{Ca}$ . Electrons added to the 3d suborbital occurs beginning with  $_{21}\text{Sc}$  and continues through  $_{30}\text{Zn}$

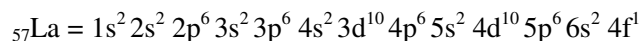


Even though the principal quantum number for 3d is lower than the principal quantum number for 4s, the latter is occupied first because the shape of the orbital allows the electron to be a fixed distance from the nucleus (in a sphere, the radius is constant), whereas the 3d suborbitals extend beyond the radius of the 4s suborbital. This inversion of orbital energy is why the transition elements are listed as B group elements in distinction from the A group elements.

(d) Fourth Cases: n = 4 means l = 0, 1, 2, 3 means m = 0, ±1, ±2, ±3 and s = ± 1/2

The 4f suborbitals begin to be filled after the 6s suborbitals. The set of quantum numbers responsible for the 4f suborbitals are:

(4, 3, 0, + 1/2) and (4, 3, 0, -1/2)  
 (4, 3, +1, + 1/2) and (4, 3, +1, -1/2)  
 (4, 3, -1, + 1/2) and (4, 3, -1, -1/2)  
 (4, 3, +2, + 1/2) and (4, 3, +2, -1/2)  
 (4, 3, -2, + 1/2) and (4, 3, -2, -1/2)  
 (4, 3, +3, + 1/2) and (4, 3, +3, -1/2)  
 (4, 3, -3, + 1/2) and (4, 3, -3, -1/2)



After the 4f suborbitals come in order by the Periodic Table: 5d, 6p, 7s, 5f, 6d, 7p  
 According to theory, all elements above atomic number 118 (with  $7p^6$ ) are inherently unstable and cannot be made.

The **Aufbau** (German for "building") **Principle** offers a way to remember the order of suborbital filling:

1s			
2s	2p		
3s	3p	3d	
4s	4p	4d	4f
5s	5p	5d	5f
6s	6p	6d	
7s	7p		

To use the Aufbau Principle, begin at 1s, then go diagonally from upper right to lower left on each successive column. In other words, suborbitals are filled in the order:

1s, 2s, 2p, 3s, 3p, 3d, 4s, 3d, 4p, 5s, 4d, 5p, 6s, 4f, 5d, 6p, 7s, 5f, 6d, 7p